

DIFFUSION MONTE CARLO CALCULATIONS FOR THE GROUND STATES OF ATOMS AND IONS IN NEUTRON STAR MAGNETIC FIELDS

S. BÜCHELER, D. ENGEL, J. MAIN and G. WUNNER*

*Institut für Theoretische Physik 1, Universität Stuttgart
70550 Stuttgart, Germany*

**E-mail: wunner@itp1.uni-stuttgart.de*

The diffusion quantum Monte Carlo method is extended to solve the old theoretical physics problem of many-electron atoms and ions in intense magnetic fields. The feature of our approach is the use of adiabatic approximation wave functions augmented by a Jastrow factor as guiding functions to initialize the quantum Monte Carlo procedure. We calculate the ground state energies of atoms and ions with nuclear charges from $Z = 2, 3, 4, \dots, 26$ for magnetic field strengths relevant for neutron stars.

Keywords: Quantum Monte Carlo; Atoms; Neutron Stars; Magnetic Fields.

1. Introduction

The discovery of features in the X-ray spectra of the thermal emission spectra of the isolated neutron star 1E 1207^{1,2} and three other isolated neutron stars has revived the interest in studies of medium- Z elements in strong magnetic fields. The reason is that the observed features could be due to atomic transitions in elements that are fusion products of the progenitor star. However, to calculate synthetic spectra for model atmospheres, and thus to be in a position to draw reliable conclusions from observed spectra to the elemental composition of the atmosphere and the distribution of elements on different ionization stages, accurate atomic data for these elements at very strong magnetic fields ($\sim 10^7$ to 10^9 T) are indispensable.

While the atomic properties of hydrogen and, partly, helium at such field strengths have been clarified in the literature over the last 25 years (for a detailed list of references see, e. g., Ref. 3), for elements with nuclear charges $Z > 2$ only fragmentary atomic data exist with an accuracy necessary for the calculations of synthetic spectra.

We have tackled³ the problem by adapting the diffusion Monte-Carlo method (DQMC)⁴⁻⁶ to the case of neutron star magnetic fields. This method has the advantage that ground-state energies can be determined practically free from approximations.

2. DQMC for neutron star magnetic fields

The basic idea of DQMC is to identify the ground state wave function $\Phi_0(\vec{R}, t)$ ($\vec{R} = (\vec{r}_1, \dots, \vec{r}_N)$) of an N -body Hamiltonian \hat{H} with a *particle density* whose correct distribution is found by following the random walk of many test particles ("walkers") in imaginary time in $3N$ -dimensional configuration space. To reduce fluctuations one works with a density distribution $f(\vec{R}, \tau) \equiv \Psi(\vec{R}, \tau)\Psi_G(\vec{R})$, where Ψ_G is a given guiding function used for importance sampling. The density distribution f obeys a drift-diffusion equation in imaginary time. Because the importance-sampled Green's function is an exponential operator, one can expand it in terms of a Euclidean path integral. For sufficiently small time steps one can write down accurate approximations to the Green's function, and sample it with diffusion Monte-Carlo.³⁻⁶

2.1. Choice of the guiding functions

The choice of the guiding function is crucial for the success of the DQMC procedure. We take the guiding function Ψ_G^{ad} as a Slater determinant of single-particle orbitals each of which is a product of a Landau state in the lowest level with a given magnetic quantum number and an unknown longitudinal wave function ("adiabatic approximation"⁷). The different longitudinal wave functions are obtained selfconsistently by an iterative solution of the Hartree-Fock equations using B-splines on finite elements.

2.2. Jastrow factor

To incorporate correlation effects it is common to multiply the guiding function by a Jastrow factor, $\Psi_G = \Psi^{\text{JF}}\Psi_G^{\text{ad}} = e^{-U(\vec{R})}\Psi_G^{\text{ad}}$. We adopt the form

$$U = -1/4 \sum_{i < j}^N r_{ij} / (1 + \sqrt{\beta} r_{ij}) + Z \sum_{i=1}^N r_i / (1 + \sqrt{\beta} r_i), \quad (1)$$

where β is the magnetic field strength in atomic units ($\beta = B/B_0$, $B_0 = 4.701 \times 10^5$ T). This leads to modifications of the adiabatic approximation guiding functions only at small distances, of the order of the Larmor radius.

3. Results and Discussion

As a representative example, Fig. 1 shows for the ground state of neutral iron ($Z = 26$) at $B = 5 \times 10^8$ T the typical flow of a diffusion quantum Monte Carlo simulation. Ions can be treated without additional complication in the same way.³ The figure depicts the energy offset E_T , the block energy E_B and the averaged block energy $\langle E_B \rangle$ as a function of the number of blocks performed.

The complete simulation goes through three stages. During the first 100 blocks, a variational quantum Monte Carlo calculation (VQMC) is performed. Since the adiabatic approximation guiding wave function is augmented by the Jastrow factor, the VQMC calculation already lowers the energy in comparison with the initial adiabatic approximation result. This stage is followed, in the next 300 blocks, by a fixed-phase diffusion quantum Monte Carlo (FPDQMC) simulation. It is seen that the onset of the simulation leads to a considerable drop in the energy. Finally, in the last 300 blocks a released-phase diffusion quantum Monte Carlo (RPDQMC) simulation is carried out, which still slightly lowers the averaged block energy, by roughly 0.1 per cent. The dashed vertical lines in Fig. 1 indicate the blocks where dynamical equilibrium of the walkers is reached. The relatively small difference between the fixed-phase and the released-phase results indicates that the phase of the adiabatic approximation wave function already well reproduces the phase of the ground state wave function. The small fluctuations of the individual block energies E_B evident in Fig. 1 are characteristic of diffusion quantum Monte Carlo simulations. It is also seen, however, that the averaged block energies $\langle E_B \rangle$ quickly converge to constant values in all three stages of the simulation. Our final RPDQMC result for the energy is $E_0 = -109.079$ keV and lies well below the density functional (DF) value. The standard deviation of the block energies at the end of the simulation in this case is $\sigma = \pm 0.186$ keV.

Table 1 lists the results for all elements from helium to iron at the magnetic field strength $B = 10^8$ T. The table contains in the first three columns the results of the three stages of the simulation and in the fourth column the energy values in adiabatic approximation calculated with our own Hartree-Fock finite-element method HFFEM. Literature values obtained by Ivanov and Schmelcher¹¹ (2DHF), by Mori and Hailey⁸ (MCPH³, multi-configurational perturbative hybrid Hartree-Hartree-Fock) and the results of density functional calculations^{9,10} (DF) are given in the remaining columns. The numbers in brackets attached to the HFFEM, 2DHF, MCPH³ and DF results designate the number of electrons occupying an

Table 1. Energy values in keV for the ground states from helium to iron at $B = 10^8$ T. Parameters of the QMC simulations: 500 walkers, time steps $\Delta\tau(Z = 2, \dots, 10) = 10^{-4}$ a.u., $\Delta\tau(Z = 11, \dots, 19) = 5 \times 10^{-5}$ a.u., $\Delta\tau(Z = 20, \dots, 26) = 2 \times 10^{-5}$ a.u. (discussion see text).

| Z | RPDQMC | FPDQMC | VQMC | HFFEM | 2DHF | MCPH ³ | DF |
|----|---------|---------|---------|------------|-----------|-------------------|----------------------|
| 2 | -0.5827 | -0.5827 | -0.5791 | -0.5754 | -0.57999 | -0.5766 | -0.6035 ^b |
| 3 | -1.230 | -1.229 | -1.220 | -1.211 | -1.22443 | -1.214 | |
| 4 | -2.081 | -2.080 | -2.065 | -2.044 | -2.07309 | -2.056 | |
| 5 | -3.122 | -3.119 | -3.095 | -3.057 | -3.10924 | -3.085 | |
| 6 | -4.338 | -4.331 | -4.294 | -4.236 | -4.31991 | -4.288 | -4.341 ^b |
| 7 | -5.716 | -5.712 | -5.660 | -5.568 | -5.69465 | -5.657 | |
| 8 | -7.252 | -7.246 | -7.173 | -7.045 | -7.22492 | -7.176 | |
| 9 | -8.938 | -8.930 | -8.834 | -8.658 | -8.90360 | -8.845 | |
| 10 | -10.766 | -10.753 | -10.630 | -10.400 | -10.72452 | -10.664 | -10.70 ^a |
| 11 | -12.725 | -12.716 | -12.569 | -12.266 | | -12.625 | |
| 12 | -14.827 | -14.817 | -14.618 | -14.249 | | -14.745 | |
| 13 | -17.061 | -17.043 | -16.813 | -16.352[1] | | -16.973[1] | |
| 14 | -19.480 | -19.461 | -19.185 | -18.619[1] | | -19.408[1] | -19.09 ^a |
| 15 | -22.022 | -22.009 | -21.665 | -21.002[1] | | -21.987[1] | |
| 16 | -24.700 | -24.668 | -24.275 | -23.482[2] | | -24.718[2] | |
| 17 | -27.541 | -27.523 | -27.044 | -26.130[2] | | -27.618[2] | |
| 18 | -30.529 | -30.509 | -29.950 | -28.890[2] | | -30.766[2] | |
| 19 | -33.650 | -33.605 | -32.999 | -31.756[2] | | -34.036[2] | |
| 20 | -36.891 | -36.881 | -36.145 | -34.750[3] | | -37.500[3] | -35.48 ^a |
| 21 | -40.296 | -40.274 | -39.458 | -37.865[3] | | | |
| 22 | -43.867 | -43.821 | -42.900 | -41.083[3] | | | |
| 23 | -47.526 | -47.490 | -46.458 | -44.426[4] | | | |
| 24 | -51.360 | -51.271 | -50.102 | -47.877[4] | | | |
| 25 | -55.279 | -55.224 | -53.915 | -51.430[5] | | | |
| 26 | -59.366 | -59.311 | -57.913 | -55.108[5] | | | -56.01 ^a |

Note: ^aRef. 9. ^bRef. 10.

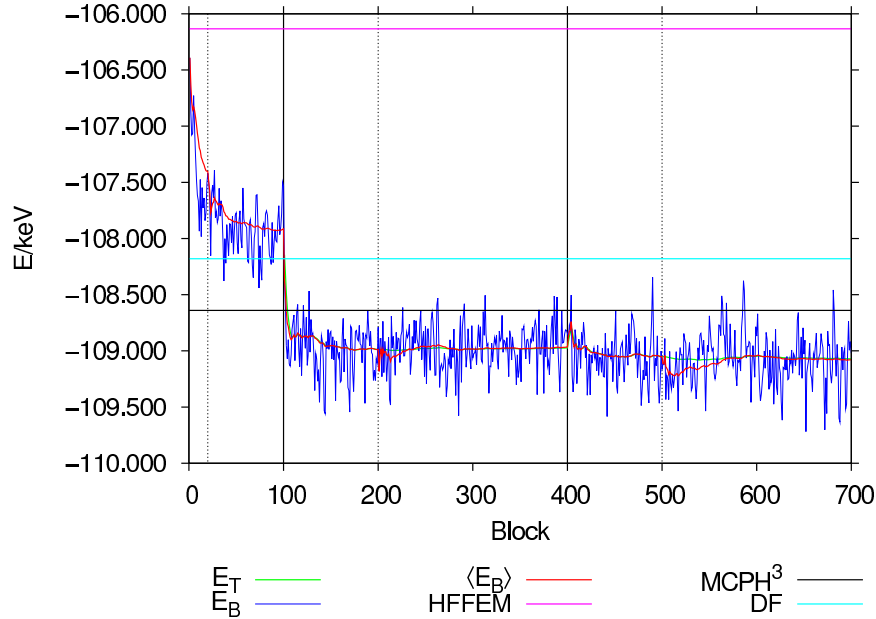


Fig. 1. Behavior of the block energy E_B (ragged curve) and the averaged block energy $\langle E_B \rangle$ (smooth curve) in the DQMC simulation for the ground state energy of neutral iron ($Z = 26$) at $B = 5 \times 10^8$ T as a function of the number of blocks. In each block, 200 time steps $\Delta\tau = 5 \times 10^{-6}$ a.u. were performed. (HFFEM (top horizontal line): energy value in adiabatic approximation; DF (second horizontal line from top): density functional result of Ref 9; MCPH³ (third horizontal line from top): result of Ref. 8.)

excited hydrogen-like single-particle longitudinal state. It can be seen that already the fixed-phase results lie slightly below the values that were obtained using the 2DHF method. The comparison with the results of the MCPH³ method shows that our RPDQMC energy values generally lie below those results, but there are also exceptions where our results lie above the MCPH³ energies. This may be due to the fact that the hybrid method is not self-consistent, since it evaluates the exchange energy in first-order perturbation theory in a basis of Hartree states and it does not include the back-reaction of the excited Landau states whose admixtures are taken into account perturbatively on the effective interaction potentials. Therefore the method need not necessarily produce an upper bound on the energy.

The comparison with the results of the DF calculations shows that these yield lower ground state energies at small nuclear charge numbers than our RPDQMC results, while for large Z the reverse is the case. The DF results

listed in Table 1 differ in the choice of the exchange functional. Given this restriction, it cannot be ensured that the DF calculations in all cases produce an upper bound on the ground state energy in magnetic fields as do the ab-initio methods used in this work or in a Ref. 11.

4. Conclusions

We have extended the released-phase diffusion Monte Carlo method to the calculation of the ground state energies of atoms and ions from helium to iron neutron star magnetic field strengths by using adiabatic approximation wave functions as guiding wave functions.³ However, for matching observed thermal spectra from isolated neutron stars, wavelength information, and thus energies of excited states, are requisite. Jones et al.⁶ have shown a way how to calculate excited states of small atoms in strong magnetic fields using the correlation function Monte Carlo method.⁵ The challenge remains to transfer their method to the DQMC simulations presented in this paper, and to calculate excited states of large atoms in intense fields.

Acknowledgments

This work was supported by Deutsche Forschungsgemeinschaft within the SFB 382 "Methods and Algorithms for Simulating Physical Processes on High-Performance Computers" at the Universities of Tübingen and Stuttgart.

References

1. D. Sanwal, G. G. Pavlov, V. E. Zavlin and A. A. Teter, *Astrophys. J.* **574**, L61 (2002).
2. S. Mereghetti, A. de Luca, P. A. Caraveo, W. Becker, R. Mignami and G. F. Bignami, *Astrophys. J.* **581**, 1280 (2002).
3. S. Bücheler, D. Engel, J. Main and G. Wunner, *Phys. Rev. A* **76**, 032501 (2007).
4. P. J. Reynolds, D. M. Ceperley, B. D. Alder and W. A. L. Jr., *J. Chem. Phys.* **77**, 5603 (1982).
5. D. M. Ceperley and B. Bernu, *J. Chem. Phys.* **89**, 6316 (1988).
6. M. D. Jones, G. Ortiz and D. M. Ceperley, *Phys. Rev. E* **55**, 6202 (1997).
7. L. I. Schiff and H. Snyder, *Phys. Rev.* **55**, 59 (1937).
8. K. Mori and C. J. Hailey, *Astrophys. J.* **564**, 914 (2002).
9. P. B. Jones, *Mon. Not. R. Astro. Soc.* **216**, 503 (1985).
10. Z. Medin and D. Lai, *Phys. Rev. A* **74**, 062507 (2006).
11. M. V. Ivanov and P. Schmelcher, *Phys. Rev. A* **61**, 022505 (2000).